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THE MACYL6 HYDRODYNAMIC CODE:

A Numerical Method for Calculating Incompressible Axisymmetric Time-Dependent Free-Surface Fluid Flows at High Reynolds Number

by

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ABSTRACT

A computer code has been developed for solving incompressible two-dimensional axisymmetric time-dependent viscous fluid flow problems involving up to two free surfaces. Heuristic models for turbulence are employed to extend the method to indefinitely high Reynolds number. Scalar quantities (heat and solute concentrations) are also followed, and the fluid may be slightly non-homogeneous in the Boussinesq approximation. The method is a second-order space, forward time explicit finite-difference scheme. Free surfaces are treated using the MAC ("Marker-and-Cell") technique.

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1. INTRODUCTION

The MACYL6 computer program was created in response to a requirement to study the events following the detonation of a nuclear device far below the surface of the sea. Of principal interest are the pulsation and upward migration under gravity of the steam bubble generated by the explosion and the resulting redistribution and upward translation of the radioactive bomb debris. The MACYL6 code, while adequate to treat the explosion problem, is also applicable to a wide variety of applied problems in various areas. It is not the purpose of the present paper to discuss such applications, but rather to describe the numerical method itself in detail. Applications to particular cases (including, of course, the explosion problem) will be published in subsequent reports.

The MACYL6 code was developed in an evolutionary fashion; an earlier and more primitive version is described in Pritchett (1967). In earlier forms, it has proved useful in the calculation of explosion phenomenology and has been successfully compared with measured field data (Pritchett and Pestaner, 1969). The latest version is a great deal more complicated than those published earlier, differing from them in two essential respects. First, scalar transport equations are introduced (in addition to the equations of fluid motion) which permit the simultaneous calculation of the space-time distributions of such quantities as temperature, salinity, bomb-debris concentration, and the like. The effects of these distributions may then be reintroduced into the fluid mechanics by allowing the fluid density to be slightly dependent on, say, temperature and salinity. This permits such effects as oceanic stability and thermohaline convection to be included in the scheme. Second, and more important, a recently-developed heuristic model for fluid turbulence is an essential part of the method. This model simulates the effects of turbulence on the flow through distributions of turbulent energy and scales of turbulence. The essential features of the model are summarized in section II; for justification, details, and comparisons with measured data the reader is referred to the original papers (Gawain and Pritchett, 1969, 1970).

The numerical method is an explicit forward-time finite-difference scheme. The momentum equation uses a nine-point second-order space difference representation of the advection terms, and the general scalar transport equation uses the more stable, but somewhat less precise "upstream" or "donor-cell" method. These are described at length in section III. The pressure-velocity (rather than the stream function-vorticity) formulation of the momentum equation is used. The MAC ("Marker-and-Cell") free-surface treatment is employed; this scheme, developed at Los Alamos (Welch, Harlow, Shannon and Daly, 1966), represents the fluid by a number of massless "marker particles" which move with the flow through the Eulerian mesh and thereby specify the position of the free surface. The treatment is in two-dimensional axisymmetric cylindrical coordinates, and the flow is assumed to be truly two-dimensional (that is, without swirl). The computer program itself is largely written in FORTRAN IV, with some portions in assembler language to increase speed; it is currently operating on Control Data 6600 equipment.

II. THE GOVERNING EQUATIONS

a. The Navier-Stokes Equations

In Eulerian coordinates (that is, coordinates fixed in space rather than moving with the flow) the equations of motion for an incompressible, homogeneous viscous fluid in a gravitational field may be written in vector notation as follows:

$$\nabla \cdot \vec{U}' = 0 \qquad \text{(II-1)}$$

$$\frac{\partial \vec{U}'}{\partial t} + \nabla \cdot (\vec{U}'\vec{U}') = -\nabla\Phi' + \upsilon\nabla^2\vec{U}' + \vec{g} \qquad \text{(II-2)}$$

where $\vec{U}'$ = velocity
Φ' = pressure/density (density being constant)
υ = fluid kinematic viscosity
$\vec{g}$ = acceleration of gravity

These equations express the principles of mass and momentum conservation, respectively. The two terms on the left of (II-2) represent the total time rate of change of momentum for an element of fluid moving with the flow. The first term on the right is the rate of momentum production due to normal pressure forces, the second expresses the rate of momentum diffusion by viscosity, and the third is the rate of momentum production by gravitational forces.

b. Scalar Transport Equations

Other transport equations which will prove useful later in the development are the transport equations for heat and solutes:

$$\frac{\partial T'}{\partial t} + \nabla \cdot (\vec{U}'T') = \kappa\nabla^2 T' + \Pi_{T'} \qquad \text{(II-3)}$$

$$\frac{\partial S'}{\partial t} + \nabla \cdot (\vec{U}'S') = C\nabla^2 S' \qquad \text{(II-4)}$$

where T' = temperature

S' = solute concentration

κ = thermal diffusivity

C = molecular diffusion coefficient

Π_T = rate of temperature change due to heat sources

The last term in equation (II-3) (the source term) will not be pursued further at this time; it represents the rate of dissipation of kinetic energy to heat.

c. <u>Turbulence and the Reynolds Stresses</u>

In incompressible flow, the equations of continuity and momentum (II-1 and II-2), along with the boundary conditions, in principle establish completely the entire fluid motion. If the flow is turbulent, however, the detailed motion, although theoretically determinate, becomes so complex that its actual calculation would involve an overwhelming amount of computation. Furthermore, in general the results of interest are certain average properties of the flow, and the large mass of additional detailed information available is usually neither required nor desired.

In Cartesian tensor notation, equations (II-1) and (II-2) may be written:

$$\frac{\partial}{\partial x_i}(U_i') = 0 \qquad \text{(II-5)}$$

$$\frac{\partial U_i'}{\partial t} + \frac{\partial}{\partial x_j}(U_i' U_j') = -\frac{\partial \Phi'}{\partial x_i} + \upsilon \frac{\partial^2 U_i'}{\partial x_j \partial x_j} + g_i \qquad \text{(II-6)}$$

If we express the total velocity and pressure fields as the sum of their mean and fluctuating components,

$$U_i' = U_i + u_i \qquad \text{(II-7)}$$

$$\Phi' = \Phi + \phi \tag{II-8}$$

(Total = mean + turbulent)

substitute these into (II-5) and (II-6) and ensemble-average the results, we obtain continuity and momentum equations for the mean flow:

$$\frac{\partial}{\partial x_i}(U_i) = 0 \tag{II-9}$$

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j}(U_i U_j) = -\frac{\partial \Phi}{\partial x_i} + g_i + \frac{\partial}{\partial x_j}\left(\nu\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \overline{u_i u_j}\right) \tag{II-10}$$

(overbars denote ensemble-averaged quantities)

Further manipulation yields an energy equation for the turbulent fluctuations:

$$\begin{aligned}\frac{\partial}{\partial t}\left(\frac{\overline{u_i u_i}}{2}\right) + \frac{\partial}{\partial x_j}\left(U_j \frac{\overline{u_i u_i}}{2}\right) = &- \frac{\overline{u_i u_j}}{2}\left(\frac{\partial U_j}{\partial x_i} + \frac{\partial U_i}{\partial x_j}\right) \\ &- \frac{\nu}{2}\overline{\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)} \\ &- \frac{\partial}{\partial x_j}\left(\overline{u_j\left(\frac{u_i u_i}{2} + \phi\right)}\right) \\ &+ \nu \frac{\partial}{\partial x_j}\left(\frac{\partial}{\partial x_j}\left[\frac{\overline{u_i u_i}}{2}\right] + \frac{\partial}{\partial x_i}\left[\overline{u_i u_j}\right]\right)\end{aligned} \tag{II-11}$$

It will be noticed that the mean flow momentum equation (II-10) resembles the original total momentum equation (II-6) except for the presence of the unknown Reynolds stresses ($-\overline{u_i u_j}$). It is customary and appropriate to postulate that these Reynolds stresses can be adequately related to the mean flow strain rates through the law:

$$-\overline{u_i u_j} = -\frac{1}{3}\overline{u_k u_k}\,\delta_{ij} + \varepsilon\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \qquad \text{(II-12)}$$

where $\delta_{ij} = 0$ for $i \neq j$ and $= 1$ for $i = j$; ε is the so-called eddy kinematic viscosity. The mean flow momentum equation is then:

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j}(U_i U_j) = -\frac{\partial P}{\partial x_i} + g_i + \frac{\partial}{\partial x_j}\left([\nu+\varepsilon]\left[\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right]\right)$$

where

(II-13)

$$P = \Phi + \frac{1}{3}\overline{u_j u_j} \qquad \text{(II-14)}$$

The above averaging process, as has been seen, results in a great simplification of the physical problem, but also involves a significant and irretrievable loss of essential information. This is apparent in the appearance of the unknown Reynolds stresses, or alternatively, of the unknown eddy viscosity distribution. To define determinate solutions, additional relations are needed. Regrettably, such supplementary relations cannot be established from the original equations (II-1) and (II-2) by any purely deductive process, and therefore empirical hypotheses are an unavoidable necessity. From another point of view, the averaged equations of motion show the effect of the Reynolds stresses on the mean flow, but the reciprocal effect of the mean flow on the Reynolds stresses is lost in the averaging process. Hence, some adequate hypothesis must be found to approximate this relationship.

For this purpose, a recently developed model for turbulent flow (Gawain and Pritchett, 1969; 1970) is used in the present work. It is similar in concept to earlier work of Prandtl (1945) and is somewhat similar to a scheme proposed at Los Alamos (Harlow and Nakayama, 1967; Hirt, 1968). Only the barest essentials of the scheme will be sketched here; for physical rationale and other details the reader is referred to the original papers.

The basic postulate in the model is that the eddy viscosity assumption (II-12) is appropriate, and that the eddy viscosity may be adequately represented by a relation of the form:

$$\varepsilon = \alpha \sqrt{\overline{u_j u_j}}\ \Lambda = \alpha \sqrt{2E}\ \Lambda \qquad \text{(II-15)}$$

where α is a slowly varying dimensionless function which may be taken as a constant outside boundary layer regions. Λ is a "scale of size" associated with the mean flow which may vary from point to point in space and time and which will be discussed later.

Combination of the basic turbulent energy equation (II-11) with the eddy viscosity postulate (II-12) yields:

$$\begin{aligned}\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}(U_j E) &= \varepsilon \Omega^2 \\ &- \frac{\upsilon}{2} \overline{\left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right)\left(\frac{\partial u_j}{\partial x_k} + \frac{\partial u_k}{\partial x_j}\right)} \\ &- \frac{\partial}{\partial x_k}\left(\overline{u_k\left[\frac{u_j u_j}{2} + \phi\right]}\right) \\ &+ \upsilon \frac{\partial}{\partial x_k}\left(\frac{\partial E}{\partial x_k} + \frac{\partial}{\partial x_j}\left[\overline{u_j u_k}\right]\right)\end{aligned} \qquad \text{(II-16)}$$

where

$$\Gamma_{jk} = \left(\frac{\partial U_j}{\partial x_k} + \frac{\partial U_k}{\partial x_j}\right) \text{ (mean flow strain rate)} \qquad \text{(II-17)}$$

$$\Omega^2 = \frac{1}{2} \Gamma_{jk} \Gamma_{jk} \qquad \text{(II-18)}$$

$$E = \frac{\overline{u_j u_j}}{2} \quad \text{(mean turbulent kinetic energy)} \qquad \text{(II-19)}$$

The terms on the right of this energy equation represent, respectively, turbulent energy production corresponding to the work done by the mean flow against the Reynolds stresses, dissipation of turbulent energy to heat, "turbulent diffusion" of energy, and molecular diffusion. In the heuristic model, the last term is neglected, as it is vanishingly small at high Reynolds numbers. The remaining terms are approximated as follows:

$$\begin{aligned} \frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}(U_j E) &= \varepsilon \Omega^2 && \text{(production)} \\ &- \upsilon \frac{2E}{\lambda^2} && \text{(dissipation)} \\ &+ \frac{\partial}{\partial x_j}\left[\gamma \varepsilon \frac{\partial E}{\partial x_j}\right] && \text{(diffusion)} \end{aligned} \qquad \text{(II-20)}$$

where λ is the so-called "dissipation length" or "turbulent microscale", and γ is another slowly varying function of the same sort as α (see equation II-15) which is constant outside boundary layers.

To complete the model, it is now only necessary to establish the "macroscale", Λ (equation II-15) and the "microscale", λ . We define a generalized mean flow strain rate Ω and a generalized mean flow strain rate gradient Ω' as follows:

$$\Omega^2 = \frac{1}{2} \Gamma_{ij} \Gamma_{ij} \qquad \text{(II-21)}$$

(see equation II-18)

$$\Omega'^2 = \left(\frac{\partial\Omega}{\partial x_i}\right)\left(\frac{\partial\Omega}{\partial x_i}\right) \qquad \text{(II-22)}$$

From these definitions, the following quantity can be obtained:

$$(\Omega\Omega')^2 = \frac{1}{4}\left(\frac{\partial\Omega^2}{\partial x_i}\right)\left(\frac{\partial\Omega^2}{\partial x_i}\right) \qquad \text{(II-23)}$$

We now define the macroscale as follows:

$$\Lambda^2(\vec{x},t) = \frac{I^2(\vec{x},t)}{J^2(\vec{x},t)} \qquad \text{(II-24)}$$

where

$$I^2(\vec{x},t) = \int_{\text{all space}} w(\vec{x},\vec{x}',t)\,\Omega^4(\vec{x}',t)\,dv' \qquad \text{(II-25)}$$

$$J^2(\vec{x},t) = \int_{\text{all space}} w(\vec{x},\vec{x}',t)\,(\Omega\Omega'(\vec{x}',t))^2\,dv' \qquad \text{(II-26)}$$

and

$$w(\vec{x},\vec{x}',t) = \frac{\exp - \left(\dfrac{(\vec{x}-\vec{x}')\cdot(\vec{x}-\vec{x}')}{\Lambda^2(\vec{x},t)}\right)}{\displaystyle\int_{\text{all space}} \exp - \left(\dfrac{(\vec{x}-\vec{x}')\cdot(\vec{x}-\vec{x}')}{\Lambda^2(\vec{x},t)}\right) dv'} \qquad \text{(II-27)}$$

Difficulty will of course be experienced in calculating the distribution directly from an arbitrary velocity distribution, since Λ appears on both sides of the defining equation. To calculate Λ explicitly, the following iteration process is used. Let the (n+1)-th approximation to Λ be defined as:

$$\Lambda^2_{n+1}(\vec{x},t) = \frac{I^2_{n+1}(\vec{x},t)}{J^2_{n+1}(\vec{x},t)} \qquad \text{(II-28)}$$

where

$$I^2_{n+1}(\vec{x},t) = \int_{\text{all space}} w_n(\vec{x},\vec{x}',t)\,\Omega^4(\vec{x}',t)\;dv' \qquad \text{(II-29)}$$

$$J^2_{n+1}(\vec{x},t) = \int_{\text{all space}} w_n(\vec{x},\vec{x}',t)\,(\Omega\Omega'(\vec{x}',t))^2 dv' \qquad \text{(II-30)}$$

and

$$w_n(\vec{x},\vec{x}',t) = \frac{\exp\left(-\dfrac{(\vec{x}-\vec{x}')\cdot(\vec{x}-\vec{x}')}{\Lambda_n^2(\vec{x},t)}\right)}{\displaystyle\int_{\text{all space}} \exp\left(-\dfrac{(\vec{x}-\vec{x}')\cdot(\vec{x}-\vec{x}')}{\Lambda_n^2(\vec{x},t)}\right) dv'} \qquad \text{(II-31)}$$

To start the iteration process, we take $\Lambda_0=\infty$ everywhere. Then in computing Λ_1, we find that the weighting function w_0 is the same everywhere, so we obtain simply:

$$\Lambda_1^2 = \frac{\displaystyle\int_{\text{all space}} \Omega^4 dv}{\displaystyle\int_{\text{all space}} (\Omega\Omega')^2 dv} \qquad \text{(II-32)}$$

a constant independent of position. Thus, Λ_2 is the first non-constant approximation to Λ that we obtain. As was discussed in the original paper, the rapid convergence of the Λ_n's justifies the approximation

$$\Lambda(\vec{x},t) \approx \Lambda_2(\vec{x},t) \qquad \text{(II-33)}$$

This procedure is also used in the present work.

The dissipation length λ is formulated as follows. Consider two lengths L_1 and L_2 defined as:

$$L_1^2 = \frac{U^2}{2E} \tag{II-34}$$

$$L_2^3 = \frac{2E}{J} \tag{II-35}$$

where J is as defined above. We now form the relation:

$$\frac{L_1 L_2}{\lambda^2} = \beta \tag{II-36}$$

where β is yet another slowly varying dimensionless function which reverts to a constant outside boundary layers. Numerical values that best match experimental data for regions outside the turbulent boundary layer are:

$$\alpha = 0.065 \tag{II-37}$$

$$\frac{1}{\beta} = 3.7 \tag{II-38}$$

$$\gamma = 1.4 \tag{II-39}$$

d. <u>Turbulent Scalar Transport</u>

As has been seen, the scalar transport equations for heat and solutes are of the form:

$$\frac{\partial Q'}{\partial t} + \frac{\partial}{\partial x_j}(U'_j Q') = C\frac{\partial^2 Q'}{\partial x_j \partial x_j} + \Pi_{Q'} \tag{II-40}$$

where Q' is the instantaneous scalar concentration, the U_j' are the instantaneous velocity components, C is a molecular diffusivity, and $\Pi_{Q'}$ is a source or sink function. These may also be expressed as the sum of mean and fluctuating components:

$$Q' = Q + q \tag{II-41}$$

$$U_j' = U_j + u_j \tag{II-42}$$

As was done for the momentum equation, the scalar transport equation may be averaged. The result is:

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x_j}(U_j Q) = \frac{\partial}{\partial x_j}\left(C\frac{\partial^2 Q}{\partial x_j} - \overline{u_j q}\right) + \Pi_Q \tag{II-43}$$

In analogy to (II-12) we postulate:

$$-\overline{u_j q} = D_T \frac{\partial Q}{\partial x_j} \tag{II-44}$$

which defines the turbulent diffusion coefficient D_T.

Although the molecular diffusivities of the various scalar quantities (such as heat, salt, etc.) may be quite different, the turbulent diffusion process is a property of the turbulence field, rather than of the particular substance being diffused. Furthermore, at high Reynolds number, it is to be expected that the turbulent diffusion coefficient will be vastly larger than the molecular diffusion coefficient. Thus, for our purpose, it is sufficient to write:

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x_j}(U_j Q) = \frac{\partial}{\partial x_j}\left(D_T \frac{\partial Q}{\partial x_j}\right) + \Pi_Q \tag{II-45}$$

We have already approximated the turbulent diffusion coefficient for turbulent kinetic energy as $\gamma\varepsilon$, where $\gamma = 1.4$. Numerous measurements (Corrsin and Uberoi, 1947; Schlicting, 1960), suggest that the "turbulent Prandtl number" (turbulent thermal diffusivity/eddy viscosity) generally takes on values between 1 and 2 for most flow situations. This suggests that it is appropriate to assume that

$$D_T = \gamma\varepsilon = 1.4\varepsilon \tag{II-46}$$

that is, that the turbulent diffusivity for turbulent energy applies to all scalar turbulent diffusion. Thus finally we obtain:

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x_j} (U_j Q) = \frac{\partial}{\partial x_j} (\gamma \varepsilon \frac{\partial Q}{\partial x_j}) + \Pi_Q \tag{II-47}$$

The source term for turbulent energy has already been defined - it is simply the work input from the mean flow minus the rate of dissipation to heat. The source term for the heat equation reflects the dissipation of both turbulent energy and mean flow kinetic energy (the latter is usually small). Thus, for heat transport, we write:

$$\frac{\partial T}{\partial t} + \frac{\partial}{\partial x_j} (U_j T) = \frac{\partial}{\partial x_j} (\gamma \varepsilon \frac{\partial T}{\partial x_j}) + \frac{\upsilon}{\sigma} (\Omega^2 + \frac{2E}{\lambda^2}) \tag{II-48}$$

where T = temperature

σ = specific heat of fluid

e. The Boussinesq Approximation

So far, we have discussed an homogeneous fluid, that is, a fluid in which the molecular viscosity and the mass density are constants. In oceanic problems however, for example, even a slight non-homogeneity in density may have profound effects upon the resulting flow. Although the density difference is quite small, the interaction of the gravitational acceleration with a slight density stratification may set up regions of stability or instability which are important in the problem. It should be pointed out, however, that density fluctuations caused by pressure fluctuations (i.e. slightly compressible behavior) are irrelevant in this regard. Only density variations due to intrinsic properties of the fluid parcel (such as temperature or salinity) have such a stabilizing or de-stabilizing effect. Therefore, rather than actual "in-situ" density, we will be concerned with "potential density": that is, density referred to some standard pressure.

Thus, we may re-write the mean-flow momentum equation in the Boussinesq approximation (retaining the density effect in the gravity term but not in the inertial terms):

$$\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j}(U_i U_j) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\upsilon+\varepsilon)\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)\right] + \xi g_i \qquad \text{(II-49)}$$

where

$$\xi = 1 + \frac{\Delta\rho}{\rho_0} = f(T,S), \quad S = \text{salinity} \qquad \text{(II-50)}$$

The salinity transport equation is simply (see II-47)

$$\frac{\partial S}{\partial t} + \frac{\partial}{\partial x_j}(U_j S) = \frac{\partial}{\partial x_j}\left(\gamma\varepsilon \frac{\partial S}{\partial x_j}\right) \qquad \text{(II-51)}$$

For seawater, for example, the dependence of potential density on salinity and temperature is well known experimentally (Knudson, 1901). For temperature in centigrade degrees and salinity in parts per thousand, over a normal range of conditions at one atmosphere the data is well represented by:

$$\begin{aligned}\rho(\text{kg/m}^3) = 1000 &- \frac{(T-3.98)^2\,(T+283)}{503.57\ (T+67.26)} \\ &+ \left[0.0634 + 1.4708\left(\frac{S-0.03}{1.805}\right) - 0.00157\left(\frac{S-0.03}{1.805}\right)^2\right. \\ &+ 0.0000398\left(\frac{S-0.03}{1.805}\right)^3\Big]\times\Big[\frac{T}{10}(18.03-0.8164T+0.01667T^2) \\ &\times\left(-0.2014+1.4708\left(\frac{S-0.03}{1.805}\right)-0.00157\left(\frac{S-0.03}{1.805}\right)^2\right. \\ &+ 0.0000398\left(\frac{S-0.03}{1.805}\right)^3\Big) + 1 - \frac{T}{1000}(4.7867-0.098185T \\ &+ 0.0010843T^2)\Big]\end{aligned} \qquad \text{(II-52)}$$

f. Summary of Principal Equations

In two-dimensional axisymmetric cylindrical coordinates, the field equations may be written as follows:

Continuity:

$$\frac{1}{r}\ \frac{\partial}{\partial r}\ (ru)\ +\ \frac{\partial v}{\partial z} = 0 \qquad \text{(II-53)}$$

Radial momentum:

$$\frac{\partial u}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}\ (ru^2)\ +\ \frac{\partial}{\partial z}\ (uv)\ =$$

$$2\left[\ \frac{1}{r}\ \frac{\partial}{\partial r}\ (r\varepsilon^*\ \frac{\partial u}{\partial r}) - \frac{\varepsilon^* u}{r^2}\ +\ \frac{\partial}{\partial z}\ (\varepsilon^*\ \frac{\partial v}{\partial r})\ \right]$$

$$+\ \frac{\partial}{\partial z}\ [\varepsilon^*(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r})\ ]$$

$$-\ \frac{\partial P}{\partial r} \qquad \text{(II-54)}$$

Vertical momentum:

$$\frac{\partial v}{\partial t} + \frac{1}{r}\ \frac{\partial}{\partial r}\ (ruv)\ +\ \frac{\partial}{\partial z}(v^2)\ =$$

$$2\ [\frac{1}{r}\ \frac{\partial}{\partial r}\ (r\varepsilon^*\ \frac{\partial u}{\partial z})\ +\ \frac{\partial}{\partial z}(\varepsilon^*\frac{\partial v}{\partial z})]$$

$$+\ \frac{1}{r}\ \frac{\partial}{\partial r}\ [r\varepsilon^*\ (\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r})]$$

$$-\ \frac{\partial P}{\partial z}\ +\ \xi g \qquad \text{(II-55)}$$

Turbulent energy:

$$\frac{\partial E}{\partial t} + \frac{1}{r}\ \frac{\partial}{\partial r}\ (ruE)\ +\ \frac{\partial}{\partial z}\ (vE)\ =\ \frac{1}{r}\ \frac{\partial}{\partial r}\ (r\gamma\varepsilon\frac{\partial E}{\partial r})\ +\ \frac{\partial}{\partial z}\ (\gamma\varepsilon\frac{\partial E}{\partial z}\ )$$

$$+\ \varepsilon\Omega^2 - \upsilon\frac{2E}{\lambda^2} \qquad \text{(II-56)}$$

Heat:

$$\frac{\partial T}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(ruT) + \frac{\partial}{\partial z}(vT) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\gamma\varepsilon\frac{\partial T}{\partial r}\right) + \frac{\partial}{\partial z}\left(\gamma\varepsilon\frac{\partial T}{\partial z}\right)$$

$$+ \frac{\upsilon}{\sigma}\left(\frac{2E}{\lambda^2} + \Omega^2\right) \qquad \text{(II-57)}$$

Salinity and/or other solutes:

$$\frac{\partial S}{\partial t} + \frac{1}{r}\frac{\partial}{\partial r}(ruS) + \frac{\partial}{\partial z}(vS) = \frac{1}{r}\frac{\partial}{\partial r}\left(r\gamma\varepsilon\frac{\partial S}{\partial r}\right) + \frac{\partial}{\partial z}\left(\gamma\varepsilon\frac{\partial S}{\partial z}\right)$$

(II-58)

where:

r = radial coordinate

z = vertical coordinate

u = radial mean flow velocity

v = vertical mean flow velocity

$\varepsilon^* = \varepsilon + \upsilon$

υ = molecular kinematic viscosity

P = total pressure

E = turbulent kinetic energy per unit mass

T = temperature

S = salinity (or other solute concentration)

ξ = density deviation parameter = $\left(1 + \frac{\Delta\rho}{\rho_0}\right)$ = prescribed function of S and T.

σ = specific heat

ε = eddy viscosity = $\alpha\sqrt{2E}\,\Lambda$

Λ = turbulent macroscale = I^2/J^2

Ω^2 = (generalized mean flow shear rate)^2 =

$$4\left[\left(\frac{\partial u}{\partial r}\right)^2 - \left(\frac{\partial u}{\partial r}\right)\left(\frac{\partial v}{\partial z}\right) + \left(\frac{\partial v}{\partial z}\right)^2\right] + \left(\frac{\partial u}{\partial z} + \frac{\partial v}{\partial r}\right)^2 \qquad \text{(II-60)}$$

$$(\Omega\Omega')^2 = \frac{1}{4}\left[\left(\frac{\partial\Omega^2}{\partial r}\right)^2 + \left(\frac{\partial\Omega^2}{\partial z}\right)^2\right] \tag{II-61}$$

$$I^2(r,z) = \frac{\iint w(r,r',z,z')\,(\Omega^2(r',z'))^2 dr'dz'}{\iint w(r,r',z,z')\; dr'dz'} \tag{II-62}$$

$$J^2(r,z) = \frac{\iint w(r,r',z,z')\,(\Omega\Omega'(r',z'))^2 dr'dz'}{\iint w(r,r',z,z')dr'dz'} \tag{II-63}$$

$$\Lambda_0^2 = \frac{\iint \Omega^4\; r\; dr\; dz}{\iint\; (\Omega\Omega')^2 r\; dr\; dz} \tag{II-64}$$

$$\lambda^2 = (\text{turbulent microscale})^2 = \frac{\upsilon}{\beta(2EJ^2)^{\gamma/6}} \tag{II-65}$$

$$w(r,r',z,z') = \sqrt{r'}\;\Psi\left(\frac{\sqrt{rr'}}{\lambda_0}\right)\; e^{-\left[\frac{(r-r')^2 + (z-z')^2}{\Lambda_0^2}\right]} \tag{II-66}$$

$$\Psi(x) = \frac{2x}{\sqrt{\pi}}\int_0^{\pi} e^{-2x^2(1-\cos\theta)}\; d\theta \tag{II-67}$$

$$\alpha = 0.065 \tag{II-68}$$

$$\frac{1}{\beta} = 3.7 \tag{11-69}$$

$$\gamma = 1.4 \tag{II-70}$$

III. THE FINITE-DIFFERENCE METHOD

a. The Computing Mesh

Consider the region of interest to be divided into a number of toroidal cells of rectangular cross-section and not-necessarily-equal cross-sectional area (see Fig. 1). If we denote a cell by the indices (i,j) where i varies with radius and j varies with height, we may establish the following nomenclature:

Δr_i = radial dimension of cell ij
Δz_j = vertical dimension of cell ij
r_i = distance from axis to center of cell ij
z_j = distance from bottom of mesh to center of cell ij
$r_{i-1/2}$ = distance from axis to inner boundary of cell ij
$r_{i+1/2}$ = distance from axis to outer boundary of cell ij
$z_{j-1/2}$ = distance from bottom of mesh to lower boundary of cell ij
$z_{j+1/2}$ = distance from bottom of mesh to upper boundary of cell ij
$\Delta r_{i-1/2}$ = distance between centers of cell ij and cell i-1 j
$\Delta r_{i+1/2}$ = distance between centers of cell ij and cell i+1 j
$\Delta z_{j-1/2}$ = distance between centers of cell ij and cell i j-1
$\Delta z_{j+1/2}$ = distance between centers of cell ij and cell i j+1

b. Continuity and Momentum

The field variables are calculated at specified points within the cell matrix as shown in Figure 2. Scalar quantities are defined at the cell center, for example P_{ij}, E_{ij}, T_{ij}, ε_{ij}, λ_{ij} and so on. The horizontal velocity component is defined at the midpoint of vertical cell faces and the vertical component at the midpoint of horizontal faces (thus we have $u_{i+\frac{1}{2}j}$, $u_{i-\frac{1}{2}j}$, $v_{ij+\frac{1}{2}j}$, $v_{ij-\frac{1}{2}}$).

The field equations (listed in section II-f) may now be written in finite-difference form. The finite-difference analogue of the mass conservation requirement (II-53) is:

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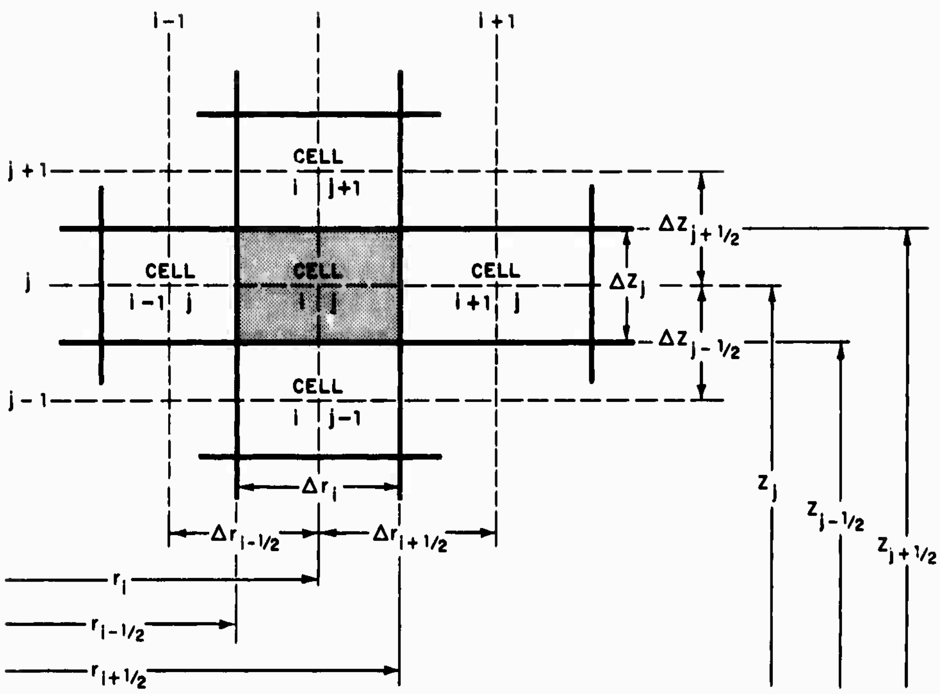

FIGURE 1: CELL NOMENCLATURE

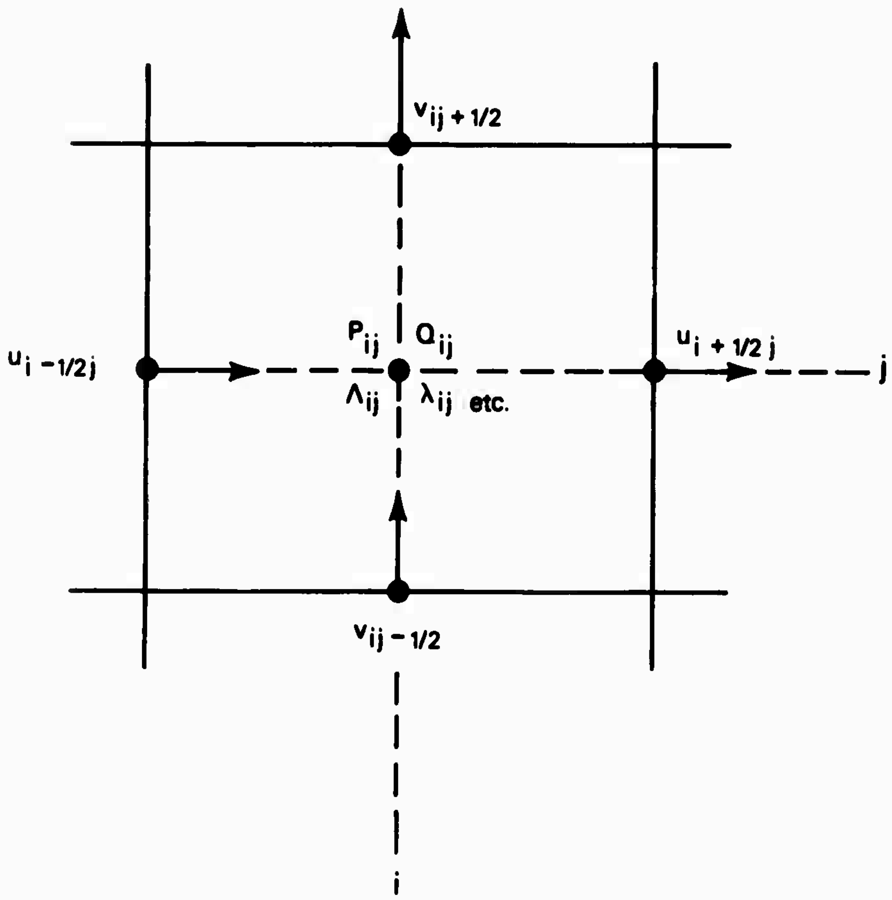

FIGURE 2: POINTS OF DEFINITION OF VARIABLES FOR CELL ij

$$D_{ij} = \text{velocity divergence in cell } ij$$

$$= \frac{1}{r_i \Delta r_i}[r_{i+\frac{1}{2}} u_{i+\frac{1}{2}j} - r_{i-\frac{1}{2}} u_{i-\frac{1}{2}j}]$$

$$+ \frac{1}{\Delta z_j}[v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}}] \qquad \text{(III-1)}$$

$$= 0$$

The radial and vertical mean flow momentum equations (II-54 and II-55) become respectively:

$$\left(\frac{\partial u}{\partial t}\right)_{i+\frac{1}{2}j} = \frac{1}{r_{i+\frac{1}{2}} \Delta r_{i+\frac{1}{2}}}[r_i (\overline{u_{ij}})^2 - r_{i+1}(\overline{u_{i+1j}})^2]$$

$$+ \frac{1}{\Delta z_j}[u^*_{i+\frac{1}{2}j-\frac{1}{2}} \overline{v_{i+\frac{1}{2}j-\frac{1}{2}}} - u^*_{i+\frac{1}{2}j+\frac{1}{2}} \overline{v_{i+\frac{1}{2}j+\frac{1}{2}}}]$$

$$+ \frac{1}{\Delta r_{i+\frac{1}{2}}}[P_{ij} - P_{i+1j}]$$

$$+ \frac{2}{r_{i+\frac{1}{2}} \Delta r_{i+\frac{1}{2}}}[\frac{r_{i+1} \varepsilon^*_{i+1j}}{\Delta r_{i+1}}(u_{i+\frac{3}{2}j} - u_{i+\frac{1}{2}j})$$

$$- \frac{r_i \varepsilon^*_{ij}}{\Delta r_i}(u_{i+\frac{1}{2}j} - u_{i-\frac{1}{2}j})]$$

$$- \frac{2\varepsilon^*_{i+\frac{1}{2}j} u_{i+\frac{1}{2}j}}{(r_{i+\frac{1}{2}})^2} + \frac{2}{\Delta z_j}[\frac{\varepsilon^*_{i+\frac{1}{2}j+\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}}$$

$$(v_{i+1j+\frac{1}{2}} - v_{ij+\frac{1}{2}}) - \frac{\varepsilon^*_{i+\frac{1}{2}j-\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}}$$

$$(v_{i+1j-\frac{1}{2}} - v_{ij-\frac{1}{2}})]$$

$$+ \frac{1}{\Delta z_j}[\varepsilon^*_{i+\frac{1}{2}j+\frac{1}{2}}(\frac{1}{\Delta z_{j+\frac{1}{2}}}(u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j})$$

(equation continued next page)

$$- \frac{1}{\Delta r_{i+\frac{1}{2}}} (v_{i+1j+\frac{1}{2}} - v_{ij+\frac{1}{2}}))$$

$$- \varepsilon^*_{i+\frac{1}{2}j-\frac{1}{2}} (\frac{1}{\Delta z_{j-\frac{1}{2}}} (u_{i+\frac{1}{2}j} - u_{i+\frac{1}{2}j-1}) - \frac{1}{\Delta r_{i+\frac{1}{2}}} (v_{i+1j-\frac{1}{2}} - v_{ij-\frac{1}{2}}))]$$

(III-2)

and

$$(\frac{\partial v}{\partial t})_{ij+\frac{1}{2}} = \frac{1}{r_i \Delta r_i} [r_{i-\frac{1}{2}} \overline{u_{i-\frac{1}{2}j+\frac{1}{2}}} v^*_{i-\frac{1}{2}j+\frac{1}{2}} - r_{i+\frac{1}{2}} \overline{u_{i+\frac{1}{2}j+\frac{1}{2}}} v^*_{i+\frac{1}{2}j+\frac{1}{2}}]$$

$$+ \frac{1}{\Delta z_{j+\frac{1}{2}}} [\overline{v_{ij}}^2 - \overline{v_{ij+1}}^2] + \frac{1}{\Delta z_{j+\frac{1}{2}}} [P_{ij} - P_{ij+1}] + \xi_{ij+\frac{1}{2}} g$$

$$+ \frac{2}{\Delta z_{j+\frac{1}{2}}} [\frac{\varepsilon^*_{ij+1}}{\Delta z_{j+1}} (v_{ij+\frac{3}{2}} - v_{ij+\frac{1}{2}}) - \frac{\varepsilon^*_{ij}}{\Delta z_j} (v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}})]$$

$$+ \frac{2}{r_i \Delta r_i} [\frac{r_{i+\frac{1}{2}} \varepsilon^*_{i+\frac{1}{2}j+\frac{1}{2}}}{\Delta z_{j+\frac{1}{2}}} (u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j})$$

$$- \frac{r_{i-\frac{1}{2}} \varepsilon^*_{i-\frac{1}{2}j+\frac{1}{2}}}{\Delta z_{j+\frac{1}{2}}} (u_{i-\frac{1}{2}j+1} - u_{i-\frac{1}{2}j})]$$

$$+ \frac{1}{r_i \Delta r_i} [r_{i+\frac{1}{2}} \varepsilon^*_{i+\frac{1}{2}j+\frac{1}{2}} (\frac{1}{\Delta r_{i+\frac{1}{2}}} (v_{i+1j+\frac{1}{2}} - v_{ij+\frac{1}{2}})$$

$$- \frac{1}{\Delta z_{j+\frac{1}{2}}} (u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j}))$$

$$- r_{i-\frac{1}{2}} \varepsilon^*_{i-\frac{1}{2}j+\frac{1}{2}} (\frac{1}{\Delta r_{i-\frac{1}{2}}} (v_{ij+\frac{1}{2}} - v_{i-1j+\frac{1}{2}})$$

$$- \frac{1}{\Delta z_{j+\frac{1}{2}}} (u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j}))] \qquad \text{(III-3)}$$

The interpolated quantities appearing in the above equations are defined as follows:

$$\overline{u_{ij}} = u_{ij}\left[\ \frac{1}{2} + \frac{1}{8}\ \left(\frac{\Delta z_{j+1}}{\Delta z_{j+\frac{1}{2}}} + \frac{\Delta z_{j-1}}{\Delta z_{j-\frac{1}{2}}}\right)\right] + u_{ij+1}\left[\ \frac{1}{8}\ \frac{\Delta z_j}{\Delta z_{j+\frac{1}{2}}}\ \right]$$

$$+\ u_{ij-1}\ \left[\frac{1}{8}\ \frac{\Delta z_j}{\Delta z_{j-\frac{1}{2}}}\ \right] \qquad \text{(III-4)}$$

$$\overline{v_{ij}} = \frac{1}{8}\ v_{ij}\ \left[\left(\frac{r_i+r_{i-\frac{1}{2}}}{r_i}\right)\left(1+\tfrac{1}{2}\ \frac{\Delta r_{i-1}}{\Delta r_{i-\frac{1}{2}}}\right) + \left(\frac{r_{i+\frac{1}{2}}+r_i}{r_i}\right)\left(2-\tfrac{1}{2}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)\right]$$

$$+\ \frac{1}{8}\ v_{i-1j}\left[\left(\frac{r_i+r_{i-\frac{1}{2}}}{r_i}\right)\left(1-\tfrac{1}{2}\ \frac{\Delta r_{i-1}}{\Delta r_{i-\frac{1}{2}}}\right)\right]$$

$$+\ \frac{1}{8}\ v_{i+1j}\left[\left(\frac{r_{i+\frac{1}{2}}+r_i}{r_i}\right)\left(\ \frac{1}{2}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)\right] \qquad \text{(III-5)}$$

where

$$u_{ij} = u_{i+\frac{1}{2}j}\left(\frac{r_{i+\frac{1}{2}}}{r_i}\ \left[1-\tfrac{1}{2}\left(\frac{r_{i+\frac{1}{2}}}{r_i} + 1\right)\right]\right) + u_{i-\frac{1}{2}j}\left(\frac{r_{i-\frac{1}{2}}}{r_i}\left[\tfrac{1}{2}\left(\frac{r_{i+\frac{1}{2}}}{r_i} + 1\right)\right]\right)$$

$$\text{(III-6)}$$

$$v_{ij} = \frac{1}{2}\ (v_{ij+\frac{1}{2}}+v_{ij-\frac{1}{2}}) \qquad \text{(III-7)}$$

and

$$\overline{u_{i+\frac{1}{2}j+\frac{1}{2}}} = u_{i+\frac{1}{2}j}\left(1-\tfrac{1}{2}\ \frac{\Delta z_j}{\Delta z_{j+\frac{1}{2}}}\right) + u_{i+\frac{1}{2}j+1}\left(\tfrac{1}{2}\ \frac{\Delta z_j}{\Delta z_{j+\frac{1}{2}}}\right)$$

$$\text{(III-8)}$$

$$\overline{v_{i+\frac{1}{2}j+\frac{1}{2}}} = \tfrac{1}{2}\ v_{ij+\frac{1}{2}}\left[\left(\frac{r_{i+\frac{1}{2}}+r_i}{r_{i+1}+r_i}\right)\left(\frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)\left(1-\ \frac{1}{4}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)\right.$$

(equation continued
next page)

$$+ \left(\frac{r_{i+1}+r_{i+\frac{1}{2}}}{r_{i+1}+r_i}\right)\left(\frac{\Delta r_{i+1}}{\Delta r_{i+\frac{1}{2}}}\right)\left(\tfrac{1}{4}\ \frac{\Delta r_{i+1}}{\Delta r_{i+\frac{1}{2}}}\right)\Big]$$

$$+ \tfrac{1}{2}v_{i+1j+\frac{1}{2}}\Big[\left(\frac{r_{i+\frac{1}{2}}+r_i}{r_{i+1}+r_i}\right)\left(\frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)\left(\tfrac{1}{4}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)$$

$$+ \left(\frac{r_{i+1}+r_{i+\frac{1}{2}}}{r_{i+1}+r_i}\right)\left(\frac{\Delta r_{i+1}}{\Delta r_{i+\frac{1}{2}}}\right)\left(1-\ \tfrac{1}{4}\ \frac{\Delta r_{i+1}}{\Delta r_{i+\frac{1}{2}}}\right)\Big] \qquad \text{(III-9)}$$

$$u^*_{i+\frac{1}{2}j+\frac{1}{2}} = \overline{u_{i+\frac{1}{2}j+\frac{1}{2}}} \qquad \text{(III-10)}$$

$$v^*_{i+\frac{1}{2}j+\frac{1}{2}} = v_{ij+\frac{1}{2}}\left(1-\tfrac{1}{2}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right) + v_{i+1j+\frac{1}{2}}\left(\tfrac{1}{2}\ \frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right)$$

$$\text{(III-11)}$$

$$4\varepsilon^*_{i+\frac{1}{2}j+\frac{1}{2}} = \varepsilon^*_{i+1j+1}\left(\frac{\Delta r_i \Delta z_j}{\Delta r_{i+\frac{1}{2}}\Delta z_{j+\frac{1}{2}}}\right) + \varepsilon^*_{i+1j}\left(\frac{\Delta r_i\ \Delta z_{j+1}}{\Delta r_{i+\frac{1}{2}}\Delta z_{j+\frac{1}{2}}}\right)$$

$$+ \varepsilon^*_{ij+1}\left(\frac{\Delta r_{i+1}\Delta z_j}{\Delta r_{i+\frac{1}{2}}\Delta z_{j+\frac{1}{2}}}\right) + \varepsilon^*_{ij}\left(\frac{\Delta r_{i+1}\Delta z_{j+1}}{\Delta r_{i+\frac{1}{2}}\Delta z_{j+\frac{1}{2}}}\right) \qquad \text{(III-12)}$$

$$2\varepsilon^*_{i+\frac{1}{2}j} = \varepsilon^*_{ij}\left(\frac{\Delta r_{i+1}}{\Delta r_{i+\frac{1}{2}}}\right) + \varepsilon^*_{i+1j}\left(\frac{\Delta r_i}{\Delta r_{i+\frac{1}{2}}}\right) \qquad \text{(III-13)}$$

$$\xi_{ij+\frac{1}{2}} = \xi_{ij}\left(\frac{\Delta z_{j+1}}{2\Delta z_{j+\frac{1}{2}}}\right) + \xi_{ij+1}\left(\frac{\Delta z_j}{2\Delta z_{j+\frac{1}{2}}}\right) \qquad \text{(III-14)}$$

Furthermore, forward time differencing will be used throughout; that is, for example,

$$u^{N+1}_{i+\frac{1}{2}j} = u^N_{ij+\frac{1}{2}} + \Delta t^{N+\frac{1}{2}}\ \left(\frac{\partial u}{\partial t}\right)^N_{i+\frac{1}{2}j} \qquad \text{(III-15)}$$

where quantities with superscript (N) are "old" values and with (N+1) "new" values; $\Delta t^{N+\frac{1}{2}}$ is the time interval between.

c. Scalar Transport

The scalar transport equations are handled somewhat differently. The general differential form for scalar transport is

$$\frac{\partial Q}{\partial t} = -\frac{1}{r}\frac{\partial}{\partial r}(r\ u\ Q) - \frac{\partial}{\partial z}(vQ) + \frac{1}{r}\frac{\partial}{\partial r}(r\gamma\varepsilon\frac{\partial Q}{\partial r}) + \frac{\partial}{\partial z}(\gamma\varepsilon\frac{\partial Q}{\partial z}) + \Pi_Q \qquad \text{(III-16)}$$

The finite difference analogue is as follows:

$$\begin{aligned}(\frac{\partial Q}{\partial t})_{ij} = {} & (\frac{1}{1-D_{ij}\Delta t^{N+\frac{1}{2}}})[\frac{1}{r_i \Delta r_i}(r_{i-\frac{1}{2}}u_{i-\frac{1}{2}j}Q^*_{i-\frac{1}{2}j} \\ & - r_{i+\frac{1}{2}}u_{i+\frac{1}{2}j}Q^*_{i+\frac{1}{2}j}) + \frac{1}{\Delta z_j}(v_{ij-\frac{1}{2}}Q^*_{ij-\frac{1}{2}} - v_{ij+\frac{1}{2}}Q^*_{ij+\frac{1}{2}})] \\ & + \frac{1}{r_i \Delta r_i}[\frac{r_{i+\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}}\gamma\varepsilon_{i+\frac{1}{2}j}(Q_{i+1j}-Q_{ij}) \\ & - \frac{r_{i-\frac{1}{2}}}{\Delta r_{i-\frac{1}{2}}}\gamma\varepsilon_{i-\frac{1}{2}j}(Q_{ij}-Q_{i-1j})] + \frac{1}{\Delta z_j}[\frac{\gamma\varepsilon_{ij+\frac{1}{2}}}{\Delta z_{j+\frac{1}{2}}}(Q_{ij+1}-Q_{ij}) \\ & - \frac{\gamma\varepsilon_{ij-\frac{1}{2}}}{\Delta z_{j-\frac{1}{2}}}(Q_{ij}-Q_{ij-1})] + \Pi_{Q_{ij}} \qquad \text{(III-17)}\end{aligned}$$

and we will again update values using forward differences:

$$Q^{N+1}_{ij} = Q^N_{ij} + t^{N+\frac{1}{2}}(\frac{\partial Q}{\partial t})^N_{ij} \qquad \text{(III-18)}$$

The velocity divergence D_{ij} (see III-1) appears in the convection terms above as part of a correction factor. In principle D_{ij} should always be identically zero, but in the calculational scheme this is not always true, and small velocity divergences may appear, as will be discussed. This correction factor tends to negate convective errors in scalar transport arising from small but finite velocity divergences.

The interpolated concentrations appearing in the convective flux terms are defined as follows:

$$\begin{aligned} Q^*_{i+\frac{1}{2}j} &= Q_{ij} && \text{if} \quad u_{i+\frac{1}{2}j} \geq 0 \\ &= Q_{i+1j} && \text{if} \quad u_{i+\frac{1}{2}j} < 0 \\ Q^*_{ij+\frac{1}{2}} &= Q_{ij} && \text{if} \quad v_{ij+\frac{1}{2}} \geq 0 \\ &= Q_{ij+1} && \text{if} \quad v_{ij+\frac{1}{2}} < 0 \end{aligned} \qquad \text{(III-19)}$$

The source terms for the various scalar quantities are as follows. For solutes, there are no sources, so:

$$\Pi_{S_{ij}} \equiv 0 \qquad \text{(III-20)}$$

For turbulent energy, we have (see II-56)

$$\Pi_{E_{ij}} = \varepsilon_{ij}\Omega^2{}_{ij} - \nu\frac{2E_{ij}}{\lambda^2{}_{ij}} \qquad \text{(III-21)}$$

and for temperature,

$$\Pi_{T_{ij}} = \frac{\nu}{\sigma}\left(\frac{2E_{ij}}{\lambda^2{}_{ij}} + \Omega^2{}_{ij}\right) \qquad \text{(III-22)}$$

where the generalized rate of mean flow shear is given by:

$$\Omega^2{}_{ij} = 4\left[\left(\frac{\partial u}{\partial r}\right)^2_{ij} - \left(\frac{\partial u}{\partial r}\right)_{ij}\left(\frac{\partial v}{\partial z}\right)_{ij} + \left(\frac{\partial v}{\partial z}\right)^2_{ij}\right]$$

$$+ \left[\left(\frac{\partial u}{\partial z}\right)_{ij} + \left(\frac{\partial v}{\partial z}\right)_{ij}\right]^2 \qquad \text{(III-23)}$$

where

$$\left(\frac{\partial u}{\partial r}\right)_{ij} = \frac{1}{\Delta r_i}\left(u_{i+\frac{1}{2}j} - u_{i-\frac{1}{2}j}\right)$$

$$\left(\frac{\partial v}{\partial z}\right)_{ij} = \frac{1}{\Delta z_j}(v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}})$$

$$\left(\frac{\partial v}{\partial r}\right)_{ij} = \frac{1}{4}\Big[\frac{1}{\Delta r_{i+\frac{1}{2}}}(v_{i+1j+\frac{1}{2}}+v_{i+1j-\frac{1}{2}}-v_{ij+\frac{1}{2}}-v_{ij-\frac{1}{2}})$$

$$-\frac{1}{\Delta r_{i-\frac{1}{2}}}(v_{i-1j+\frac{1}{2}}+v_{i-1j-\frac{1}{2}}-v_{ij+\frac{1}{2}}-v_{ij-\frac{1}{2}})\Big]$$

$$\left(\frac{\partial u}{\partial z}\right)_{ij} = \frac{1}{4}\Big[\frac{1}{\Delta z_{j+\frac{1}{2}}}(u_{i+\frac{1}{2}j+1}+u_{i-\frac{1}{2}j+1}-u_{i+\frac{1}{2}j}-u_{i-\frac{1}{2}j})$$

$$-\frac{1}{\Delta z_{j-\frac{1}{2}}}(u_{i+\frac{1}{2}j-1}+u_{i-\frac{1}{2}j-1}-u_{i+\frac{1}{2}j}-u_{i-\frac{1}{2}j})\Big]$$

d. <u>Turbulent Mixing</u>

To establish the eddy viscosity distribution we must first fix the distribution of the macroscale Λ, which in turn depends on certain space integrals of Ω^2 (defined above) and the quantity $(\Omega\Omega')^2$ as discussed in section II-c. This latter quantity is expressed in finite-difference form as follows:

$$4(\Omega\Omega')^2_{ij} = \frac{(\Omega^2_{i+1j} - \Omega^2_{i-1j})^2}{(\Delta r_{i+\frac{1}{2}} + \Delta r_{i-\frac{1}{2}})^2} + \frac{(\Omega^2_{ij+1} - \Omega^2_{ij-1})^2}{(\Delta z_{j+\frac{1}{2}}+\Delta z_{j-\frac{1}{2}})^2} \qquad \text{(III-24)}$$

The "averaging distance" Λ_0 may now be formed as:

$$\Lambda_0^2 = \frac{\sum\limits_{i}^{\text{all cells}}\sum\limits_{j} (\Omega^2_{ij})\, r_i \Delta r_i \Delta z_j}{\sum\limits_{i}^{\text{all cells}}\sum\limits_{j} (\Omega\Omega')^2_{ij}\, r_i \Delta r_i \Delta z_j} \qquad \text{(III-25)}$$

and the "characteristic integrals" I^2 and J^2 are:

$$I^2_{ij} = \frac{\overset{\text{all cells}}{\sum_{i'}\sum_{j'}} w_{i,i',j,j'} \left(\Omega^2_{i'j'}\right)^2}{\overset{\text{all cells}}{\sum_{i'}\sum_{j'}} w_{i,i',j,j'}} \qquad \text{(III-26)}$$

$$J^2_{ij} = \frac{\overset{\text{all cells}}{\sum_{i'}\sum_{j'}} w_{i,i',j,j'} \left(\Omega\Omega'^2_{i'j'}\right)}{\overset{\text{all cells}}{\sum_{i'}\sum_{j'}} w_{i,i',j,j'}} \qquad \text{(III-27)}$$

where

$$w_{i,\ i',\ j,\ j'} =$$

$$\sqrt{r_{i'}}\ \Psi\left(\frac{r_i r_{i'}}{\lambda_0}\right) e^{-\left[\frac{(r_{i'} - r_i)^2 + (z_{j'} - z_j)^2}{\Lambda_0^2}\right]} \Delta r_i \Delta z_j \qquad \text{(III-28)}$$

and $\Psi(x)$ is defined in equation (II-67); it is illustrated in Figure 3. Now, the "scales of size" may be formed. The "microscale" or "dissipation length" is just:

$$\lambda^2_{ij} = \frac{\upsilon}{\beta(2E_{ij}J^2_{ij})^{1/6}} \qquad \text{(III-29)}$$

and the macroscale is:

$$\Lambda^2_{ij} = I^2_{ij}/J^2_{ij} \qquad \text{(III-30)}$$

whence:

$$\varepsilon_{ij} = \alpha\sqrt{2E_{ij}}\ \Lambda_{ij} \qquad \text{(III-31)}$$

e. <u>Explicit Solution for Pressure</u>

Examination of the preceding field equations shows that, if the entire set of velocities and Q's is known, the changes in these velocities and Q's over a short time interval can be calculated. The only missing quantity is the pressure distribution (P_{ij}). In incompressible flow, the pressure distribution may be found from the mass conservation constraint ($\nabla \cdot \vec{u} = 0$). We first write an expression for the time rate of change of the velocity divergence in cell ij;

$$\frac{D_{ij}^{N+1} - D_{ij}^{N}}{\Delta t^{N+\frac{1}{2}}} = \frac{1}{r_i \Delta r_i} \left[r_{i+\frac{1}{2}} \left(\frac{\partial u}{\partial t}\right)^N_{i+\frac{1}{2}j} - r_{i-\frac{1}{2}} \left(\frac{\partial u}{\partial t}\right)^N_{i-\frac{1}{2}j} \right]$$

$$+ \frac{1}{\Delta z_j} \left[\left(\frac{\partial v}{\partial t}\right)^N_{ij+\frac{1}{2}} - \left(\frac{\partial v}{\partial t}\right)^N_{ij-\frac{1}{2}} \right] \qquad \text{(III-32)}$$

If the finite-difference momentum equations (III-2 and III-3) are substituted into this expression, considerable cancellation occurs, and the result is:

$$\frac{D_{ij}^{N+1} - D_{ij}^{N}}{\Delta t^{N+\frac{1}{2}}} = \left\{ \frac{1}{r_i \Delta r_i} \left[\frac{r_{i+\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}} (P_{ij} - P_{i+1j}) \right.\right.$$

$$\left. + \frac{r_{i-\frac{1}{2}}}{\Delta r_{i-\frac{1}{2}}} (P_{ij} - P_{i-1j}) \right] + \frac{1}{\Delta z_j} \left[\frac{1}{\Delta z_{j+\frac{1}{2}}} (P_{ij} - P_{ij+1}) \right.$$

$$\left.\left. \frac{1}{\Delta z_{j-\frac{1}{2}}} (P_{ij} - P_{ij-1}) \right] + \zeta_{ij} \right\}^N \qquad \text{(III-33)}$$

where ζ_{ij} =

$$\frac{1}{r_i \Delta r_i} \left[\frac{1}{\Delta r_{i+\frac{1}{2}}} \left(r_i \overline{u_{ij}}^2 - r_{i+1} \overline{u_{i+1j}}^2 \right) + \frac{1}{\Delta r_{i-\frac{1}{2}}} \left(r_i \overline{u_{ij}}^2 - r_{i-1} \overline{u_{i-1j}}^2 \right) \right]$$

$$+ \frac{1}{\Delta z_j} \left[\frac{1}{\Delta z_{j+\frac{1}{2}}} \left(\overline{v_{ij}}^2 - \overline{v_{ij+1}}^2 \right) + \frac{1}{\Delta z_{j-\frac{1}{2}}} \left(\overline{v_{ij}}^2 - \overline{v_{ij-1}}^2 \right) \right]$$

(Equation continued on next page)

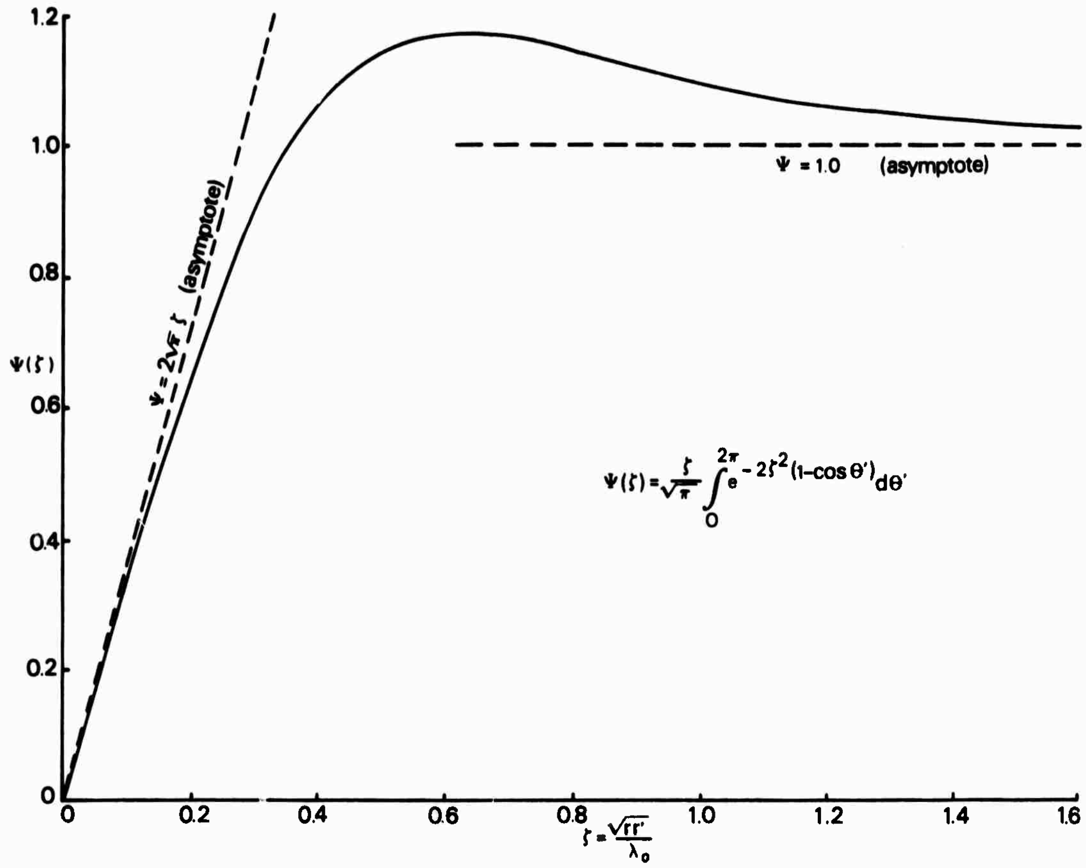

FIGURE 3 THE GEOMETRIC FUNCTION Ψ

FIGURE 3: THE GEOMETRIC FUNCTION Ψ

$$+ \frac{1}{r_i \Delta r_i \Delta z_j} [r_{i+\frac{1}{2}} ([u^* \bar{v} + \bar{u} v^*]_{i+\frac{1}{2} j-\frac{1}{2}} - [u^* \bar{v} + \bar{u} v^*]_{i+\frac{1}{2} j+\frac{1}{2}})$$

$$+ r_{i-\frac{1}{2}} ([u^* \bar{v} + \bar{u} v^*]_{i-\frac{1}{2} j+\frac{1}{2}} - [u^* \bar{v} + \bar{u} v^*]_{i-\frac{1}{2} j-\frac{1}{2}})]$$

$$+ \frac{g}{2\Delta z_j} [\xi_{ij} (\frac{\Delta z_{j+1}}{\Delta z_{j+\frac{1}{2}}} - \frac{\Delta z_{j-1}}{\Delta z_{j-\frac{1}{2}}}) + \xi_{ij+1} (\frac{\Delta z_j}{\Delta z_{j+\frac{1}{2}}}) - \xi_{ij-1} (\frac{\Delta z_j}{\Delta z_{j-\frac{1}{2}}})]$$

$$+ \varepsilon^*_{i+1j} [\frac{2r_{i+1}}{r_i \Delta r_i \Delta r_{i+\frac{1}{2}} \Delta r_{i+1}} (u_{i+\frac{3}{2} j} - u_{i+\frac{1}{2} j})]$$

$$+ \varepsilon^*_{i-1\ j} [\frac{2r_{i-1}}{r_i \Delta r_i \Delta r_{i-\frac{1}{2}} \Delta r_{i-1}} (u_{i-\frac{1}{2} j} - u_{i-\frac{3}{2} j})]$$

$$+ \varepsilon^*_{ij+1} [\frac{2}{\Delta z_j \Delta z_{j+\frac{1}{2}} \Delta z_{j+1}} (v_{ij+\frac{3}{2}} - v_{ij+\frac{1}{2}})]$$

$$+ \varepsilon^*_{ij-1} [\frac{2}{\Delta z_j \Delta z_{j-\frac{1}{2}} \Delta z_{j-1}} (v_{ij-\frac{1}{2}} - v_{ij-\frac{3}{2}})]$$

$$- \varepsilon^*_{ij} [\frac{2}{(\Delta r_i)^2} (u_{i+\frac{1}{2} j} - u_{i-\frac{1}{2} j}) (\frac{1}{\Delta r_{i-\frac{1}{2}}} + \frac{1}{\Delta r_{i+\frac{1}{2}}})$$

$$+ \frac{2}{(\Delta z_j)} (v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}}) (\frac{1}{\Delta z_{j-\frac{1}{2}}} + \frac{1}{\Delta z_{j+\frac{1}{2}}})]$$

$$+ \varepsilon^*_{i-\frac{1}{2} j} [\frac{2u_{i-\frac{1}{2} j}}{r_i \Delta r_i \Delta r_{i-\frac{1}{2}}}] - \varepsilon^*_{i+\frac{1}{2} j} [\frac{2u_{i+\frac{1}{2} j}}{r_i \Delta r_i \Delta r_{i+\frac{1}{2}}}]$$

$$+ \varepsilon^*_{i+\frac{1}{2} j+\frac{1}{2}} [\frac{2r_{i+\frac{1}{2}}}{r_i \Delta r_i \Delta z_j} (\frac{u_{i+\frac{1}{2} j+1} - u_{i+\frac{1}{2} j}}{\Delta z_{j+\frac{1}{2}}} + \frac{v_{i+1 j+\frac{1}{2}} - v_{ij+\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}})]$$

$$+ \varepsilon^*_{i-\frac{1}{2} j-\frac{1}{2}} [\frac{2r_{i-\frac{1}{2}}}{r_i \Delta r_i \Delta z_j} (\frac{u_{i-\frac{1}{2} j} - u_{i-\frac{1}{2} j-1}}{\Delta z_{j-\frac{1}{2}}} + \frac{v_{ij-\frac{1}{2}} - v_{i-1 j-\frac{1}{2}}}{\Delta r_{i-\frac{1}{2}}})]$$

$$- \varepsilon^*_{i+\frac{1}{2} j-\frac{1}{2}} [\frac{2r_{i+\frac{1}{2}}}{r_i \Delta r_i \Delta z_j} (\frac{u_{i+\frac{1}{2} j} - u_{i+\frac{1}{2} j-1}}{\Delta z_{j-\frac{1}{2}}} + \frac{v_{i+1 j-\frac{1}{2}} - v_{ij-\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}})]$$

$$- \varepsilon^*_{i-\frac{1}{2} j+\frac{1}{2}} [\frac{2r_{i-\frac{1}{2}}}{r_i \Delta r_i \Delta z_j} (\frac{u_{i-\frac{1}{2} j+1} - u_{i-\frac{1}{2} j}}{\Delta z_{j+\frac{1}{2}}} + \frac{v_{ij+\frac{1}{2}} - v_{i-1 j+\frac{1}{2}}}{\Delta r_{i-\frac{1}{2}}})]$$

(III-34)

The pressure equation is obtained by setting D_{ij}^{N+1} (the "new" value) equal to zero. This is a "self-correcting" feature of the method; even if at some time large divergences do exist, they will be quickly eliminated. That is, we arrange the rate of change of D_{ij} so as to tend to "zero out" D_{ij}^{N+1}. Therefore, the pressure equation is:

$$\frac{1}{r_i \Delta r_i} \left[\frac{r_{i+\frac{1}{2}}}{\Delta r_{i+\frac{1}{2}}} (P_{ij}-P_{i+1j}) + \frac{r_{i-\frac{1}{2}}}{\Delta r_{i-\frac{1}{2}}} (P_{ij}-P_{i-1j}) \right]$$

$$+ \frac{1}{\Delta z_j} \left[\frac{1}{\Delta z_{j+\frac{1}{2}}} (P_{ij}-P_{ij+1}) + \frac{1}{\Delta z_{j-\frac{1}{2}}} (P_{ij}-P_{ij-1}) \right]$$

$$+ R_{ij} = 0 \qquad \text{(III-35)}$$

where

$$R_{ij} = \zeta_{ij} + \frac{D_{ij}^{N}}{\Delta t^{N+\frac{1}{2}}} \qquad \text{(III-36)}$$

Note that R_{ij} contains only velocities, eddy viscosities, and ξg's. Therefore, if we are given a set of these variables, equation III-35 may be solved by an iterative technique for the pressure field.

IV. BOUNDARY CONDITIONS

a. Fixed Walls

The computing mesh is bounded within an upright circular cylinder, whose walls are rigid and impermeable. These walls are considered to be "free-slip" - that is, along a wall, the velocity component normal to the wall must be zero, but the tangential component is not constrained. This is justified since we are primarily concerned with problems at high Reynolds number, and it is to be expected that the boundary layer thickness will be negligibly small compared to the grid resolution. This "tank" may be of arbitrary diameter and height, so that boundary effects may be minimized by moving the boundary far away; on the other hand, boundary effects may be of interest (for example, the effect of a nearby sea bottom upon the behavior of an underwater explosion bubble). For convenience, we will designate the boundaries as the "wall", "ceiling", "floor", and "axis". The axis, of course, does not represent a true physical boundary, but is rather an axis of symmetry. However, boundary conditions appropriate for a physical boundary are also appropriate here.

The finite-difference equations when applied to cell ij require quantities located in neighboring cells; it is therefore necessary to add one layer of cells outside each boundary (see Figure 4). The boundary conditions are then applied by inserting values for the field variables in these fictitious cells at each time step such that the boundary conditions are satisfied. The field equations provide exactly the information required to obtain these relations. For simplicity (and without loss of generality) we use:

$$\Delta r_1 = \Delta r_2$$
$$\Delta r_M = \Delta r_{M-1}$$
$$\Delta z_1 = \Delta z_2$$
$$\Delta z_N = \Delta z_{N-1}$$

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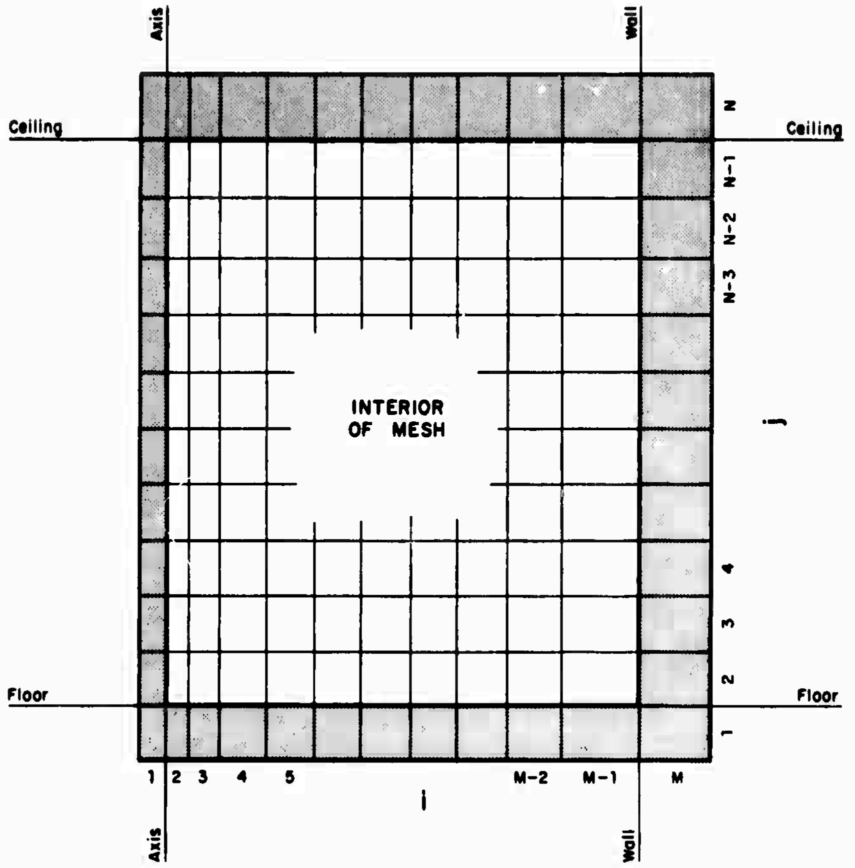

FIGURE 4: LAYOUT OF THE COMPUTING MESH

where i = 1 is the layer "on the other side" of the axis, i = M is the layer outside the wall, j = 1 is the layer under the floor, and j = N is the layer above the ceiling. In general, the boundary conditions are that no flux of transported scalars (whether convective or diffusive) may occur through a boundary, and that the velocity constraint mentioned earlier applies. These will be satisfied if the following obtains:

Axis:
$$\begin{aligned} u_{\frac{1}{2}j} &= -u_{2\,\frac{1}{2}j} \\ v_{1j+\frac{1}{2}} &= v_{2j+\frac{1}{2}} \\ u_{1\frac{1}{2}j} &= 0 \\ P_{1j} &= P_{2j} \\ \varepsilon_{1j} &= \varepsilon_{2j} \\ Q_{1j} &= Q_{2j} \end{aligned} \qquad \text{(IV-1)}$$

Floor:

$$\begin{aligned} u_{i+\frac{1}{2}\,1} &= u_{i+\frac{1}{2}\,2} \\ v_{i1\,\frac{1}{2}} &= 0 \\ v_{i\,\frac{1}{2}} &= -v_{i2\,\frac{1}{2}} \\ P_{i\,1} &= P_{i2}-\xi_{i2}g\Delta z_1 \\ \varepsilon_{i\,1} &= \varepsilon_{i2} \\ Q_{i\,1} &= Q_{i2} \\ \xi_{i\,1} &= \xi_{i2} \end{aligned} \qquad \text{(IV-2)}$$

Ceiling:

$$\begin{aligned} u_{i+\frac{1}{2}N} &= u_{i+\frac{1}{2}N-1} \\ v_{iN-\frac{1}{2}} &= 0 \\ v_{iN+\frac{1}{2}} &= -v_{iN-\frac{3}{2}} \end{aligned}$$

(Equation continued)

$$P_{iN} = P_{iN-1} + \xi_{iN-1} g \Delta z_N \tag{IV-3}$$

$$\varepsilon_{iN} = \varepsilon_{iN-1}$$

$$Q_{iN} = Q_{iN-1}$$

$$\xi_{iN} = \xi_{iN-1}$$

Wall:

$$u_{M+\frac{1}{2}j} = -\frac{r_M r_{M-\frac{3}{2}}}{r_{M+\frac{1}{2}} r_{M-1}} u_{M-\frac{3}{2}j}$$

$$u_{M-\frac{1}{2}j} = 0$$

$$v_{Mj+\frac{1}{2}} = v_{M-1j+\frac{1}{2}} \tag{IV-4}$$

$$P_{Mj} = P_{M-1j}$$

$$+ u^2_{M-\frac{3}{2}j} \left(\frac{r_{M-\frac{3}{2}}}{r_{M-1}}\right)^2 \left[\frac{r_{M-1}}{r_{M-\frac{1}{2}}} \left(\tfrac{1}{4}\left(\frac{r_{M-\frac{1}{2}}}{r_{M-1}} + 1\right)\right)^2\right.$$

$$\left. - \frac{r_M}{r_{M-\frac{1}{2}}} \left(1 - \tfrac{1}{4}\left(\frac{r_{M+\frac{1}{2}}}{r_M} + 1\right)\right)^2\right]$$

$$\varepsilon_{Mj} = \varepsilon_{M-1j}$$

$$Q_{Mj} = Q_{M-1j}$$

where Q is E, T, or S.

b. Free Surfaces

The boundary conditions at a free surface may be summarized as follows:

1) There must be no stress tangential to the surface.
2) Pressure must be continuous across the surface.
3) There must be no Q transport through the surface.

The problem is, where are these conditions to be applied, or rather, how are free surfaces to be located within the mesh? In order to identify which portion of the mesh is filled with fluid and which portion is empty, we insert a number of massless "marker particles" which move with the fluid and which participate in the calculation only to the extent that they allow the computer to "flag" cells as full or empty. In particular, at the end of a time step, each particle is moved with a velocity which is interpolated between adjacent principal velocity points in the mesh. That is, designating the coordinate of particle k as $\tilde{r}_k$, $\tilde{z}_k$:

For $r_i \leq \tilde{r}_k < r_{i+1}$ and $z_{j-\frac{1}{2}} \leq \tilde{z}_k < z_{j+\frac{1}{2}}$,

$$
\begin{aligned}
\tilde{v}_k = {} & v_{ij-\frac{1}{2}} \\
& + \left(\frac{\tilde{z}_k - z_{j-\frac{1}{2}}}{\Delta z_j}\right)(v_{ij+\frac{1}{2}} - v_{ij-\frac{1}{2}}) \\
& + \left(\frac{\tilde{r}_k - r_i}{\Delta r_{i+\frac{1}{2}}}\right)\left(\frac{\tilde{z}_k - z_{j-\frac{1}{2}}}{\Delta z_j}\right)(v_{i+1j+\frac{1}{2}} - v_{ij+\frac{1}{2}}) \\
& + \left(1 - \frac{\tilde{z}_k - z_{j-\frac{1}{2}}}{\Delta z_j}\right)\left(\frac{\tilde{r}_k - r_i}{\Delta r_{i+\frac{1}{2}}}\right)(v_{i+1j-\frac{1}{2}} - v_{ij-\frac{1}{2}})
\end{aligned}
$$

and for

$$
r_{i-\frac{1}{2}} \leq \tilde{r}_k < r_{i+\frac{1}{2}} \quad , \quad z_j \leq \tilde{z}_k < z_{j+1} \;, \tag{IV-5}
$$

$$
\begin{aligned}
\tilde{u}_k = {} & \left(u_{i+\frac{1}{2}j} + \frac{\tilde{z}_k - z_j}{\Delta z_{j+\frac{1}{2}}}(u_{i+\frac{1}{2}j+1} - u_{i+\frac{1}{2}j})\right) \\
& \left(\frac{r_{i+\frac{1}{2}}}{\tilde{r}_k}\left[1 - \frac{(r_{i+\frac{1}{2}} + \tilde{r}_k)(r_{i+\frac{1}{2}} - \tilde{r}_k)}{2 r_i \Delta r_i}\right]\right) \\
& + \left(u_{i-\frac{1}{2}j} + \frac{\tilde{z}_k - z_j}{\Delta z_{j+\frac{1}{2}}}[u_{i-\frac{1}{2}j+1} - u_{i-\frac{1}{2}j}]\right)\left(\frac{r_{i-\frac{1}{2}}}{\tilde{r}_k}\left[\frac{(r_{i+\frac{1}{2}} + \tilde{r}_k)(r_{i+\frac{1}{2}} - \tilde{r}_k)}{2 r_i \Delta r_i}\right]\right)
\end{aligned} \tag{IV-6}
$$

Then, we replace:

$$\tilde{r}_k^{N+1} = \tilde{r}_k^{N} + \tilde{u}_k^{N+1} \Delta t^{N+\frac{1}{2}} \tag{IV-7}$$

$$\tilde{z}_k^{N+1} = \tilde{z}_k^{N} + \tilde{v}_k^{N+1} \Delta t^{N+\frac{1}{2}} \tag{IV-8}$$

Two sorts of void, the air and the bubble, are allowed for in the scheme, and therefore we have two free surfaces. Cell status is assigned by the flagging of each cell in one of five ways:

AIR: The cell is empty (contains no particles) and is in the region designated as air.

BUB: The cell contains no particles and is within the bubble.

AIRSUR: The cell contains particles, but is directly adjacent to at least one AIR cell.

BUBSUR: The cell contains particles, but is directly adjacent to at least one BUB cell.

FULL: The cell contains particles, and all adjacent cells also contain particles, i.e. are either FULL, AIRSUR, or BUBSUR.

Note: "Adjacent" in the above context means "sharing a side with" - diagonal relationships are not considered.

Thus, at the beginning of a problem, each cell is flagged in one of the above ways. At the end of each time cycle, the particles are moved, and the cells reflagged if necessary. A typical arrangement of particles and cell flags is shown in Figure 5. Only certain transitions are permitted, however - for example, a cell previously flagged as FULL may not, in one cycle, change to an AIR cell. This rule is to prevent the spontaneous opening of voids deep within the fluid due to the happenstance that the cell should momentarily contain no particles. To become an AIR cell, a FULL cell must first pass through AIRSUR status. These transition rules are summarized in Figure 6.

One other pathological condition can occur, however. A cell may attempt to become an AIRSUR and a BUBSUR cell simultaneously - that is, it contains particles, but is faced on one side with an AIR cell and on the other by a BUB cell. What is done when, and if, this occurs is to assume that the bubble has "leaked"; the layer of fluid between the air and the bubble has become less than one cell thick. Computationally, when this condition is detected, all BUB and BUBSUR cells are subsequently re-designated AIR and AIRSUR cells respectively. It should be pointed out, in passing, that there is no requirement that there be a bubble involved in the problem at all - the MACYL scheme can handle single-surface problems as well as two-surface ones.

The application of the boundary conditions is fairly straightforward, once the flags are known on each cell. For pressure, we merely say that the pressure in an AIR or AIRSUR cell is simply P_A (an input constant) and that in a BUB or BUBSUR cell is P_B (an arbitrary function of bubble volume and/or time). For velocities in surface cells of either type, if one side is "open", the requirement that $D_{ij} = 0$ supplies the missing value. If more than one side is open, we require that

$$\frac{1}{r}\frac{\partial}{\partial r}(ru) = 0$$

$$\frac{\partial v}{\partial z} = 0$$

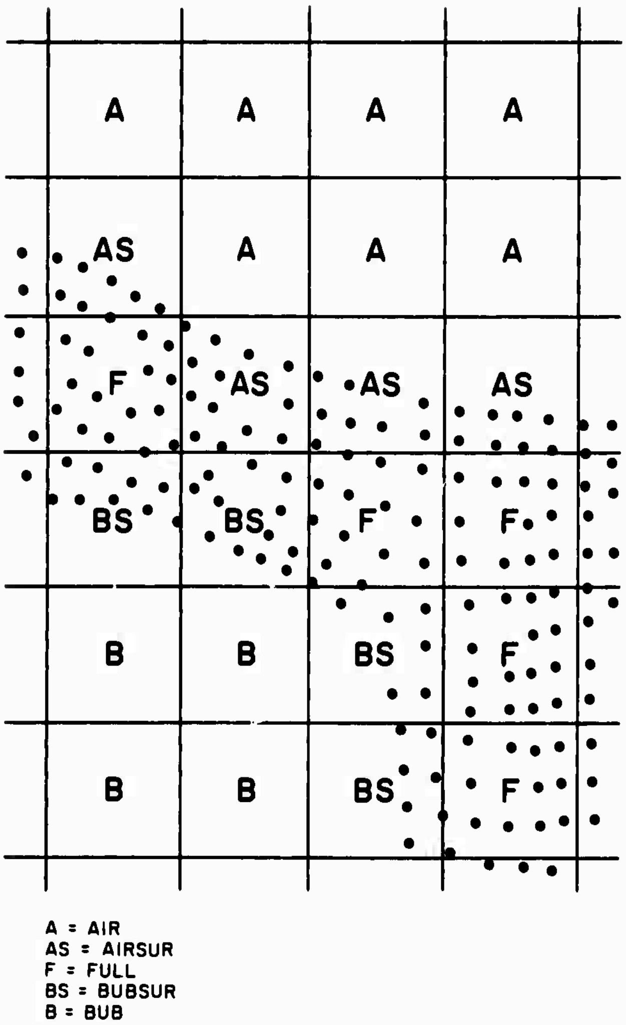

FIGURE 5: CELL FLAGS

separately (this is analogous to the treatment in <u>Welch et. al</u>., 1966). Note that a cell with all four sides open contains fluid which is simply in a gravitational trajectory.

CYCLE N

CYCLE N + 1	AIR	AIRSUR	FULL	BUBSUR	BUB
AIR	YES	YES	NO	NO	NO
AIRSUR	YES	YES	YES	YES	NO
FULL	NO	YES	YES	YES	NO
BUBSUR	NO	YES	YES	YES	YES
BUB	NO	NO	NO	YES	YES

FIGURE 6: CELL FLAG TRANSITION RULES

V. STABILITY AND ACCURACY

As is true of finite-difference schemes in general, the MACYL code must contend with potential numerical instability. These instabilities are intrinsic in the finite resolution of the space-time grid, and in general may be found by a comparison of the finite-difference equations with the original differential equations using, for example, Taylor expansions. The first (and most obvious) restriction is the incompressible analogue of the Courant condition, which arises from the convection terms in the equations:

$$\Delta t << \frac{\Delta X}{|\vec{u}|} \quad \text{everywhere} \tag{V-1}$$

where ΔX is a space interval, and $\vec{u}$ is a velocity, (either a material velocity or a gravity wave phase velocity). Thus we obtain two requirements:

$$\Delta t << \frac{\Delta X}{U_{max}} \tag{V-2}$$

$$\Delta t << \sqrt{\left|\frac{2\pi(\Delta X)^2}{g\ W \tanh(2\pi H/W)}\right|} \tag{V-3}$$

where

U_{MAX} = maximum material velocity

W = longest gravity wavelength present (usually the mesh diameter)

H = maximum fluid depth

Physically, this means that no disturbance is allowed to traverse more than one cell in a single time step. Numerical experiments suggest that adequate accuracy can be maintained if we require that:

$$\Delta t \leq 0.4 \; \frac{\Delta X}{|\vec{u}|_{max}} \qquad \text{(V-4)}$$

Another constraint on the time step relates to rates of diffusion. To prevent instability, we must require that:

$$\Delta t \;\; << \;\; \frac{(\Delta X)^2}{\varepsilon^*} \qquad \text{everywhere} \qquad \text{(V-5)}$$

Actually, this requirement will only be important when diffusive effects dominate convective effects: for the class of problems of interest here, (V-1) will generally override (V-5). To maximize efficiency, at the end of each time cycle, we calculate the maximum time step consistent with numerical stability and use it for the next interval.

Still another requirement relates to the value of the eddy viscosity. This requirement arises from high-order errors in the convection terms of the finite-difference representation of the momentum equations. These high-order errors are of a diffusive character, and the "artificial diffusivity" thus created may be of either sign. We require that:

$$\varepsilon \geq \; |c(\Delta X)^2 \Omega| \qquad \text{(V-6)}$$

where $c \approx 0.7$. If the eddy viscosity at a particular space-time point is not large enough to satisfy (V-6), we "boost" the eddy viscosity so as to just satisfy the requirement. It should be noted, however, that this "boosting" occurs only in the "vorticity-diffusion" terms of the momentum equation. That is, the turbulent-plus-viscous terms in the momentum equations are of the form:

r-direction:

$$2\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon^{*}\frac{\partial u}{\partial r}\right) - \frac{\varepsilon u^{*}}{r^{2}} + \frac{\partial}{\partial z}\left(\varepsilon^{*}\frac{\partial v}{\partial z}\right)\right]$$

$$+ \frac{\partial}{\partial z}\left[\varepsilon^{*\prime}\left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right)\right]$$

z-direction:

$$2\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\varepsilon^{*}\frac{\partial u}{\partial z}\right) + \frac{\partial}{\partial z}\left(\varepsilon^{*}\frac{\partial v}{\partial z}\right)\right]$$

$$+ \frac{1}{r}\frac{\partial}{\partial r}\left[r\,\varepsilon^{*\prime}\left(\frac{\partial u}{\partial z} - \frac{\partial v}{\partial r}\right)\right]$$

and the boosted viscosity only appears in the finite-difference analogues of the equations where indicated by $\varepsilon^{*\prime}$. Violations of this requirement tend to generate spurious wave-like disturbances or vortices of wavelength one computational cell.

One test of the accuracy of the method is whether or not transported quantities (momentum, salinity, etc.) are conserved rigorously. It may be shown directly from the finite-difference equations that this is so, and therefore the error is of order computer round-off error (about 10^{-15}). Another test of any incompressible scheme is whether mass, or fluid volume, is conserved. If D_{ij} were always exactly zero, this would be true by definition. As has been shown however, it is not generally zero, but only of very small magnitude (D_{ij} may, of course, be made arbitrarily small by "tightening" the convergence criterion in the pressure iteration procedure). Another way of checking on mass conservation is to keep track of the total fluid volume as the calculation proceeds. There is a slight ambiguity here, however. The problem is, for a surface cell, how much of the cell is considered to be full of fluid?

Somewhat arbitrarily, the following rules were chosen to evaluate the best estimate of the fluid volume in a surface cell:

1) If the cell is open on one side only, or on two opposite sides, it is considered to be half-full.

2) Otherwise, it is considered one-quarter full.

Naturally, total volumes calculated in this way fluctuate slightly from cycle to cycle due to the surface ambiguity. The amplitude of the fluctuation decreases, of course, as resolution is increased. It has been shown, however, that even for problems carried out through thousands of time cycles, the mean of the fluctuating values does not shift, but remains the same throughout the calculation. Therefore, the small D_{ij}'s are in some sense randomly distributed, and their effects cancel.

VI. THE COMPUTER PROGRAM

The necessary tools have now been developed to assemble a procedure for solution. If, at time t, we know the entire state of the system, we may update the field variables to their values at $t+\Delta t$ through the following procedure:

Step 1 - Calculate and store values of R_{ij} (defined by equations III-34 III-36) for all FULL cells.

Step 2 - Iterate a solution for the entire pressure field in FULL cells using a Gauss-Seidel iteration procedure in connection with equation III-35 until the entire P_{ij} field converges. The criterion for convergence is:

$$\frac{\left| {}^{k}P_{ij} - {}^{k-1}P_{ij} \right|}{\left| {}^{k}P_{ij} \right| + \left| {}^{k-1}P_{ij} \right| + u_{ij}^{2} + v_{ij}^{2} + |gH| + \left| P_A - P_B \right|} < 10^{-4}$$

for all ij

where superscripts k-1, k denote successive passes through the iteration loop, and H is the maximum fluid depth expected in the problem.

Step 3 - Calculate new velocities based on the new set of pressures, the momentum equations (III-2 and -3), and the boundary conditions discussed in section IV.

Step 4 - Calculate and store values for the quantities $\Omega^2{}_{ij}$ and $(\Omega\Omega')^2{}_{ij}$ for all FULL, AIRSUR and BUBSUR cells (III-23,-24).

Step 5 - Compute the "averaging distance" Λ_0 per equation III-25.

Step 6 - Calculate the "macroscale" (Λ_{ij}) and "microscale" (λ_{ij}) distributions for all FULL, AIRSUR, and BUBSUR cells as outlined in equations III-26 through III-30.

Step 7 - Evaluate the eddy viscosity distribution (ε_{ij}) in all FULL, AIRSUR, and BUBSUR cells (III-31).

Step 8 Update time ($t^{N+1} = t^N + \Delta t^{N+\frac{1}{2}}$); calculate a new time interval based on stability requirements V-4 and V-5; output the state of the system.

Step 9 Update E_{ij} (the turbulent energy distribution) using equations III-17 and III-21.

Step 10 Update the temperature distribution (the T_{ij}'s) using equations III-17 and III-22.

Step 11 Update solute concentrations using III-17 and III-20. The program allows for two solute fields; one is usually salinity, and the other may be used to follow a dissolved contaminant.

Step 12 Re-evaluate ξ_{ij} for all FULL, AIRSUR and BUBSUR cells using the new T_{ij}'s and S_{ij}'s, and the appropriate "equation of state" for the fluid (such as equation II-52 for seawater).

Step 13 Move the marker particles according to IV-5, -6, -7, and -8.

Step 14 Reflag cells as required, as discussed in section IV-b; re-evaluate P_B (the bubble pressure) and return to step 1.

VII. CONCLUSIONS

The MACYL6 computer program is currently operating on the CDC 6600 computing system at the Lawrence Radiation Laboratory in Berkeley, California. As has been discussed, earlier versions of the scheme have been checked against both analytic solutions and experimental data, with favorable results; in general, the agreement with data is within error of measurement. The program will shortly be put to work in an investigation of the explosion debris transport from very deep underwater nuclear explosions. The potential of the scheme for application to other problems associated with underwater explosions, as well as oceanographic and meteorological problems in general, appears to be great.

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APPENDIX - LIST OF SYMBOLS

C	molecular diffusion coefficient
D_{ij}	velocity divergence in cell ij
E	Turbulent kinetic energy per unit mass
e	2.71828...
$\vec{g}$	acceleration of gravity (vector)
g	vertical component of acceleration of gravity
H	maximum fluid depth expected in problem
i,j,k	Part II: Cartesian tensor indices (subscripts)
i,j	Part III: *et seq.*: space grid indices in r, z directions respectively (subscripts)
I^2	first characteristic integral
J^2	second characteristic integral
M	maximum value of i index (denotes "wall") (subscript)
N	maximum value of j index (denotes "ceiling") (subscript)
N,N+1	integer index denoting time step (superscript)
P	mean total pressure = $\Phi + \frac{2}{3}E$
P_A	air pressure
P_B	bubble pressure
Q'	instantaneous generalized scalar concentration
Q	mean generalized scalar concentration
q	turbulent generalized scalar concentration fluctuation
R_{ij}	$\zeta_{ij} + D_{ij}/\Delta t$
r	radial coordinate
$r_{i+\frac{1}{2}}$	radial coordinate of center of cell ij
r_i	radial coordinate of outer boundary of cell ij
$\tilde{r}_k$	radial coordinate of particle k
S'	instantaneous salinity (or solute concentration)
S	mean salinity (or solute concentration)

T'	instantaneous temperature
T	mean temperature
t	time
$\vec{U}'$	instantaneous velocity (vector)
$\vec{U}$	mean velocity (vector)
$\vec{u}$	turbulent velocity fluctuation (vector)
u	radial velocity
$\tilde{u}_k$	radial velocity of particle k
v	vertical velocity
$\tilde{v}_k$	vertical velocity of particle k
W	longest gravity wavelength present
w	weighting function
ΔX	generalized space interval
z	vertical coordinate
z_j	vertical coordinate of center of cell ij
$z_{j+\frac{1}{2}}$	vertical coordinate of upper boundary of cell ij
$\tilde{z}_k$	vertical coordinate of particle k
$\left.\begin{matrix}\alpha\\ \beta\\ \gamma\end{matrix}\right\}$	turbulence model functions
Γ_{ij}	mean flow strain rate tensor
δ_{ij}	Kroeneker delta function
∂	denotes partial differentiation
Δ	denotes a finite difference or interval
∇	vector nabla operator
ε	eddy viscosity
ε^*	$\varepsilon + \upsilon$
ζ_{ij}	$(\nabla^2 P)_{ij}$
κ	molecular thermal diffusivity

$\Lambda_0, \Lambda_1, ..$ successive approximations to Λ

Λ	turbulent macroscale
λ	turbulent microscale
υ	kinematic viscosity
ξ	density variation factor = $1 + \frac{\Delta\rho}{\rho_0}$
Π_Q	source term for scalar quantity Q
π	3.14159265...
ρ	fluid density
σ	specific heat
Φ'	instantaneous pressure
Φ	mean pressure
ϕ	turbulent pressure fluctuation
Ψ	geometric function for cylindrical coordinates
Ω	generalized mean flow strain rate
Ω'	generalized mean flow strain rate gradient

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ERRATA

IRA-TR-1-70, "The MACYL6 Hydrodynamic Code: A Numerical Method for Calculating Incompressible Axisymmetric Time-Dependent Free-Surface Fluid Flows at High Reynolds Number," by John W. Pritchett, 15 May 1970.

p. 9: sentence after Eq. (II-27) should read:

"Difficulty will of course be experienced in calculating the Λ distribution...."

p. 12: Eq. (II-43) should read:

$$\frac{\partial Q}{\partial t} + \frac{\partial}{\partial x_j}(U_j Q) = \frac{\partial}{\partial x_j}\left(C \frac{\partial Q}{\partial x_j} - \overline{u_j q}\right) + \Pi_Q$$